Ground-state properties of the infinite-range vector spin-glasses

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The ground-state properties of the infinite-range vector spin-glasses are studied by a "slow-cooling" iterative solution of the mean-field equations. Results are presented for the zero-temperature probability distribution $P(H)$ of internal fields with and without an external magnetic field present. We also find the ground-state energy for the XY and Heisenberg models. $P(H)$ has a hole; i.e., $P(H) = 0$ for $H < H_0$, which persists in high magnetic fields and relatively high temperatures, $T/T_c \lesssim \frac{1}{2}$. Our studies for the infinite-range Heisenberg spin-glass appear to show macroscopic irreversibility, in contrast to the short-range Heisenberg case which has no irreversibility. Therefore the range of interaction plays an important role in determining the irreversible behavior.

Considerable progress has recently been made in understanding the nonergodic[1-4] behavior of the infinite-range Ising spin-glass model of Sherrington and Kirkpatrick[5] (SK). However, little progress has been made in understanding the irreversible and time-dependent effects for this model. Theoretical studies[6,7] of the infinite-range, isotropic Heisenberg model using replica techniques find a spin-glass phase at a well-defined transition temperature T_c. Below T_c, the replica symmetry has been shown to be broken. Though the breaking of replica symmetry is often presumed to be related to irreversibility and the onset of history-dependent effects, there is presently no proof that these phenomena are connected. It is the purpose of this paper to explore the irreversibility and metastable properties of the infinite-range, vector spin-glasses.

Recently, it was demonstrated[8,9] that the mimina of the free-energy surface as functions of temperature T and the external field H could explain the nature of reversible and irreversible behavior in *short-range* Ising and Heisenberg spin-glasses. A very striking result[9] in that in an *isotropic* Heisenberg spin-glass there is no irreversibility. The field-cooled (FC) and zero-field–cooled (ZFC) states are found to be the same, and magnetic hysteresis is absent. These results at first sight seem to be in conflict with those of Refs. 6 and 7, if we make the (as yet unproved) connection between replica symmetry breaking and the onset of irreversibility. However, since the calculations are for an infinite-ranged model it is important to study the reversibility or irreversibility of the long-ranged vector models.

In the present paper we study the ground-state properties and check whether there is irreversibility in the infinite-range vector spin-glasses. We employ iterative mean-field theory[8,9] to study the ground-state properties.

We calculate the N dependence of the ground-state energies for the infinite-range spin-glasses as well as the probability distributions of internal magnetic fields with and without an external magnetic field present. We compare our results with those of the Monte Carlo (MC) method,[10] and find agreement (wherever MC results exist). However, our method,[8,9] as we will discuss below, is a factor of 10–100 faster than MC. We also find that the infinite-range Heisenberg spin-glass for $N \geq 400$ shows irreversibility below T_c.

The SK model[5] generalized to vector spins is described by the Hamiltonian

$$H = -\sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j - \sum_i \vec{h} \cdot \vec{S}_i \tag{1}$$

for N classical spins S_i, where $\vec{h}$ is the external magnetic field. The summation is over all pairs (ij). The exchange interactions (J_{ij}) are given by the Gaussian distribution

$$P(J_{ij}) = \left[\frac{N-1}{2\pi} \right]^{1/2} J^{-1} \exp[-(N-1)J_{ij}^2/2J^2] \ . \tag{2}$$

The spins may be m-component vectors or Ising-like $(S_i = \pm 1)$ but, in either case, $|S_i| = 1$. A particular sample has a fixed set J_{ij} of the $N(N-1)/2$ values of J_{ij} which are chosen randomly from a Gaussian probability distribution of zero mean and variance $J^2/(N-1)$. We take $J = 1$. The N dependence of the interactions ensures a correct thermodynamic limit. We have scaled J by the number of neighbors $N - 1$. In the limit $N \to \infty$ one usually replaces $N - 1$ by N, but for the small sample studied here this difference is noticeable.

As discussed previously[8,9] the reaction term in the free-energy functional $F[\vec{m}_i]$, where $\vec{m}_i$ is the thermal average of the vector spin at the ith site, leads to unphysical minima to which the system will readily flow. Here we are mainly interested in the $T = 0$ results, in which case the reaction term vanishes. Consequently, we can consider only the mean-field terms. A major advantage of our mean-field approach is that the metastability or variational condition $\delta F/\delta m_i = 0$ can be solved by simple iterative techniques[8,9] for fixed H and T. All states so generated are minima of the free-energy surface.[8,9] They can be readily followed with H and T. Because no matrix algebra is required we can treat fairly large systems.

We solve iteratively the self-consistent equations deriving from $\delta F/\delta \vec{m}_i = 0$,

$$\vec{m}_i = \frac{\vec{h}_i}{|h_i|} S B_S(|h_i|) \ , \tag{3}$$

where $\vec{h}_i = \sum_i J_{ij} \vec{m}_j + \vec{h}$ and B_S is the Brillouin function for general spin S. Here we choose $S = 1$. Convergence is as-

sumed when

$$\frac{\sum_i [(\vec{m}_i)_n - (\vec{m}_i)_{n-1}]^2}{\sum_i (\vec{m}_i)_n^2} \leq 10^{-8} \ , \tag{4}$$

where the subscript n denotes the nth iteration. In most cases we begin our numerical calculations at high $T \cong 1.5 T_c$, where T_c is the mean-field spin-glass transition temperature, and cool in zero or finite field. The iterations at high T are started by choosing the direction of the $\vec{m}_i$ randomly. The temperature is then decreased in small steps, typically 0.1 or $0.2 J$. At each temperature we could follow the solution with decreasing T without difficulty. At each subsequent T, the converged values of the previous temperature were used to start the next iteration. In this way it is assumed that the system "follows" a given minimum of the energy surface as it evolves in H and T. As in most numerical approaches, we take advantage of the fact that updating the $\vec{m}_i$ as we iterate leads to much more rapid convergence.

Our results for the N dependence of the ground-state energy per particle N of the infinite-range XY and Heisenberg spin-glasses are shown in Fig. 1. These results are also summarized in Table I. Note that $1/\sqrt{N}$ dependence of E/N is well obeyed for both cases. The results for the XY model agree with the MC results of Palmer and Pond,[10] except at very small N where the difference is significant. This difference is due to the different normalization of J. We normalize with $N-1$ while Palmer and Pond use N. The major improvement over the earlier work is that the "slow cooling" iterative solution of the mean-field equation is considerably faster[8,9] (by a factor of 10–100) than the MC techniques.

It has been shown by Bray and Moore[11] that the number of metastable minima for the infinite-range spin-glass grows very rapidly with N. For $N \geq 200$ for the XY model and $N \geq 400$ for the Heisenberg model, the number of metastable states is large and one should expect to have problems finding the true ground state. We found that for large N the states that one obtains by a slow cooling MC procedure or by slowly cooling the mean-field equations are not necessarily the lowest and therefore we have to do other
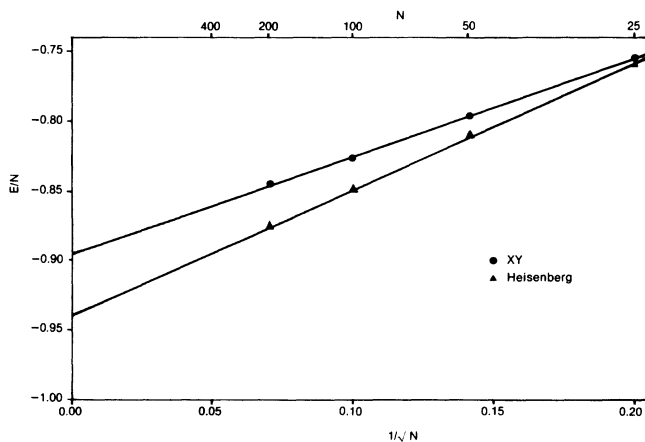

FIG. 1. Ground-state energies plotted vs $1/\sqrt{N}$. The solid points are for the xy model and the solid triangles are for the Heisenberg system. Error bars are less than the size of the points.

TABLE I. Ground-state energy for the infinite range XY and Heisenberg spin-glass model. N is the number of spins and M is the number of $[J_{ij}]$ configurations which were averaged over.

| | | E/N | |
N	M	XY	Heisenberg
25	200	-0.755 ± 0.004	-0.759 ± 0.003
50	200	-0.797 ± 0.002	-0.810 ± 0.002
100	100	-0.826 ± 0.002	-0.850 ± 0.002
200	50	-0.8435 ± 0.002	-0.8755 ± 0.002
∞		-0.895 ± 0.010	-0.940 ± 0.010

"tricks"[10] to obtain the global minimum. For this reason we have calculated E/N only for N in which the number of minima is small and where we believe we have the lowest-energy state. The $1/\sqrt{N}$ extrapolation suggests that $(E/N)_\infty = -0.895 \pm 0.010$ for the XY case, compared with -0.904 ± 0.014 that Palmer and Pond[10] give from their MC work. Because the mean-field procedure for obtaining ground-state energies is faster than the MC technique we have for the first time been able to determine the N dependence of the ground-state energy for the infinite-range Heisenberg spin-glass. For the Heisenberg case we also find that the data follow a $1/\sqrt{N}$ dependence reasonably well. We find $(E/N)_\infty = -0.94 \pm 0.01$ from the $1/\sqrt{N}$ extrapolation. Not surprisingly, the energy as $N \rightarrow \infty$ is appreciably lower than the Ising model and slightly lower than the XY model, as would be expected because of the additional degrees of freedom. Indeed, we expect the energy to decrease steadily with increasing number of spin components, eventually reaching the spherical model[12] limit $(E/N)_\infty = -1$.

In Fig. 2 we present our results for the internal-field distributions for the XY model and Heisenberg model. For a given sample, the average internal field projected along the direction $\vec{m}_i$ is

$$H_i = \sum_j J_{ij} \vec{m}_i \cdot \vec{m}_j + \vec{h} \cdot \vec{m}_i \ , \tag{5}$$

where $\vec{h}$ is the external field. The $P(H)$ histograms of Fig. 2 for $N = 200$ were averaged over $M = 100$ samples for the XY model and 50 for the Heisenberg model. Note that these histograms are the $T = 0$ results, where the mean-field theory is exact. In particular, our results for the XY model for $h = 0$ agree very well with the MC results of Palmer and Pond.[10] As is clearly shown in Fig. 2(a) the $P(H)$ distribution has a hole, no spins feel an internal field for $H \leq 0.585$ in agreement with Ref. 10. $P(H)$ does not change considerably even with the application of an external field of $h = J$. The size of the hole remains essentially unchanged. The major effect of h is near the maximum in $P(H)$, where the introduction of h shifts the upper cutoff to higher H. In Fig. 2(b) we present our results for $P(H)$ for the Heisenberg case. Results for 400 spins in the Heisenberg model were essentially the same, with less finite size rounding at H_0, the lower limit of $P(H)$. We know of no MC results for the Heisenberg case with which to compare these results. Our results are in very good agreement with earlier theoretical calculations of $P(H)$ for the XY and Heisenberg spin-glasses by Bray and Moore.[13] As expected, $P(H)$ has
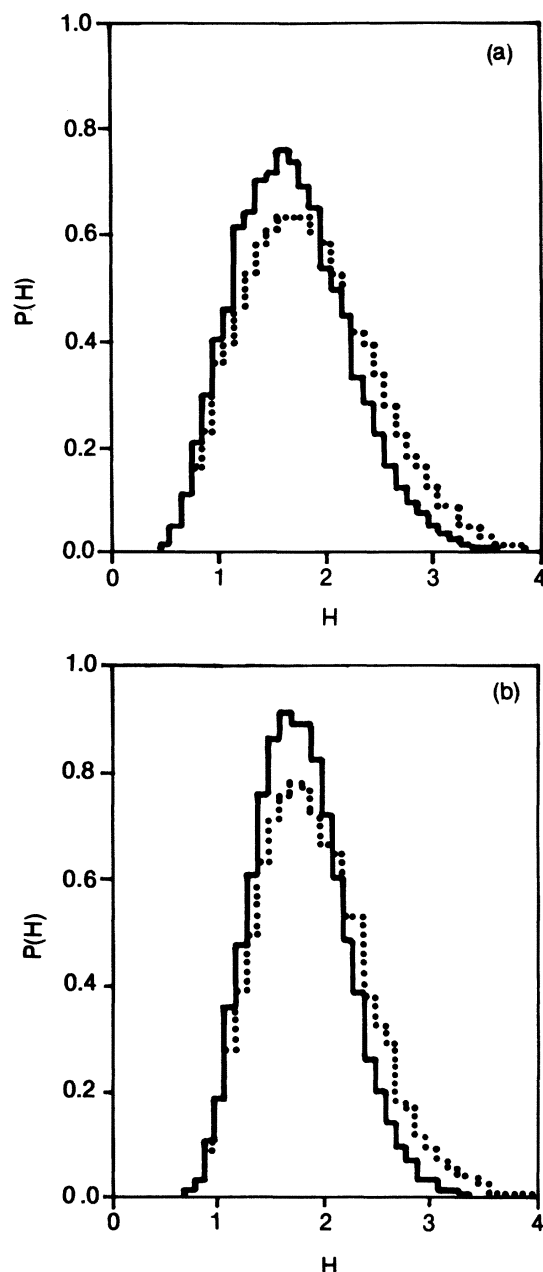
FIG. 2. Histograms of the internal field distribution in an (a) XY spin-glass and (b) Heisenberg spin-glass. The solid line indicates results for zero external field and the dotted histogram for $h = 1.0$ J. Each histogram is an average of 100 samples of 200 spins for the XY model and 50 samples for the Heisenberg model.

a hole for the Heisenberg model. The size of the hole is $H_0 = 0.85$, slightly larger than for the XY case. In the Heisenberg case $P(H)$ becomes sharper and the width of $P(H)$ at half maximum is smaller than the XY case. In this case the width at half maximum is 0.90, which agrees favorably with the theoretical result of Bray and Moore[13] which gives 0.93. For the XY case the width is 1.25 for both theory[13] and simulation. The introduction of an external magnetic field in the Heisenberg case has exactly the same effect as in the XY case, i.e., the size of hole remains essentially unchanged but the maximum in $P(H)$ moves to higher H.

In Fig. 3 we plot $P(H)$ with $h = 0$ for the Heisenberg model for three temperatures.[14] These results are obtained by iteratively solving the mean-field equations for $N = 200$ spins and averaging over $M = 50$ configurations. Note that the hole in the $P(H)$ is still present even when $T = 0.5$, where $T_c = 1.3$ from our mean-field theory.[15] It is interesting that the hole in $P(H)$ is still present even when only the mean-field theory equations, which ignore fluctuations, are used. Similar results are also found for the XY model. Therefore, to obtain the hole in $P(H)$ for the vector infinite-range spin-glasses, one does not need the equations of Thouless, Anderson, and Palmer.[10] Of course, as temperature is increased, $P(H)$ moves to lower H as expected, since many of the spins feel a lower internal field.

Finally, we looked very carefully for reversible and irreversible effects in the infinite-range vector spin-glasses. This is a very interesting problem to address, since our previous observations[8,9] for the short-range Heisenberg spin-glass[9] is that there is no macroscopic irreversibility. We have systematically looked for irreversibility in the infinite-range spin-glasses. By cooling to almost zero temperature in the presence of a small magnetic field $(h = 0.1)$, we can calculate the FC magnetization (M^{FC}). However, by cooling slowly from high T to very low T in the presence of zero external field and then applying the field, we can calculate the ZFC magnetization. For $N < 200$ spins there is no irreversibility $(M^{FC} = M^{ZFC})$ but, for $N \geq 400$, irreversibility $(M^{FC} \neq M^{ZFC})$ appears to exist. We studied six different configurations of J_{ij} for $N = 400$, half of them showed irreversible behavior and half did not. For small N $(N \leq 200)$ the number of metastable states for a Heisenberg infinite-range spin-glass is very small (less than 5) and the dispersion of the energies of the metastable states is also small. Therefore, by calculating the FC and ZFC magnetizations for small external field $(h = 0.1)$ we always found reversibility, i.e., $M^{FC} = M^{ZFC}$. As we increase the number
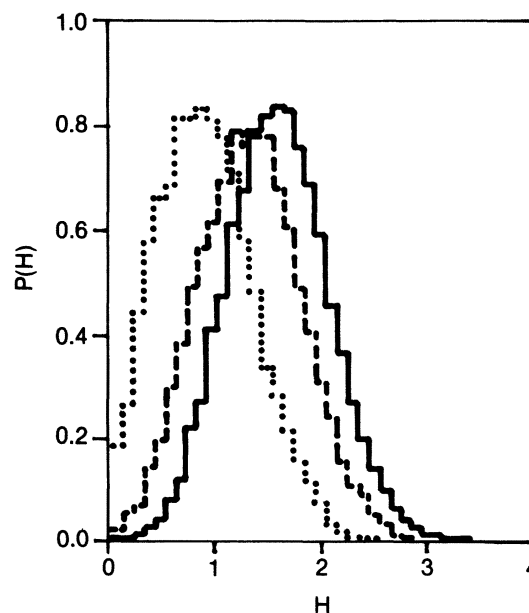

FIG. 3. Histograms of the internal field distribution for a Heisenberg spin-glass at three different temperatures. Solid line is for $T = 0.5$, dashed line for $T = 0.7$, and dotted line for $T = 0.9$, where $T_c = 1.3$. Each histogram is an average of 50 samples of 200 spins.

of spins $(N = 400)$ there are enough metastable states[11] $(\sim 28$ for $H = 0)$ and enough dispersion for the energies of metastable states[11] that we see irreversibility, $M^{FC} \neq M^{ZFC}$. Even in those samples which were reversible for both $N = 200$ and 400, the number of iterations necessary to minima hop to the new ground state after the field is switched on is large, usually of order 300 moves per spin. The large number of iterations are suggestive of the fact that the system had to make many macroscopic rearrangements. Since the total number of metastable minima is still small for $N \leq 400$, it often fell into the lowest-energy state. For N large the system will not be able to find the lowest-energy state and it will be irreversible. Therefore our results for the infinite-range Heisenberg spin-glass suggest that irreversibility exists for large N. The range of interactions plays an important role in determining the characteristics of irreversible processes. It seems that the barriers between minima become larger as the range of interaction increases and the lowest-energy state is not as accessible as in the finite-range case.

To conclude, we have studied the internal-field distribution with and without an external magnetic field at $T = 0$ for the infinite-range *vector* spin-glasses. The knowledge of the internal-field distribution plays a very important part in the understanding of the low-temperature properties of spin-glasses. We also show that the infinite-range spin-glass shows macroscopic irreversibility even for the Heisenberg case, suggesting that the range of interaction plays an important role in determining the reversible behavior in spin-glasses. Finally, we note that this work is another example of how the slow cooling iterative solution of the mean-field equations[8,9] can help to obtain results for the ground-state properties of the infinite-range vector spin-glasses, which would require significantly more computer time to obtain similar results with regular Monte Carlo techniques.

[1]A. P. Young and S. Kirkpatrick, Phys. Rev. B 25, 440 (1982); A. P. Young and S. Jain, J. Phys. A 16, L199 (1983).
[2]H. Sompolinsky, Phys. Rev. Lett. 47, 935 (1981).
[3]N. O. Mackenzie and A. P. Young, Phys. Rev. Lett. 49, 301 (1983).
[4]F. T. Bantilan and R. G. Palmer, J. Phys. F 11, 261 (1981).
[5]D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. 35, 1792 (1975); Phys. Rev. B 17, 4384 (1978).
[6]M. Gabay and G. Toulouse, Phys. Rev. Lett. 47, 201 (1981).
[7]D. M. Cragg, D. Sherrington, and M. Gabay, Phys. Rev. Lett. 49, 158 (1982).
[8]C. M. Soukoulis, K. Levin, and G. S. Grest, Phys. Rev. Lett. 48, 1756 (1983); Phys. Rev. B 28, 1495 (1983).
[9]C. M. Soukoulis, G. S. Grest, and K. Levin, Phys. Rev. Lett. 50, 80 (1983); Phys. Rev. B 28, 1510 (1983).
[10]R. G. Palmer and C. M. Pond, J. Phys. F 9, 1451 (1979).

[11]A. J. Bray and M. A. Moore, J. Phys. C 15, 2417 (1982). The number of metastable states for the infinite-range spin-glass is given by $\exp(Ng)$ where $g = 0.20$ for Ising spins, 0.023 for XY spins, and 0.0084 for Heisenberg spins. N is the number of spins.
[12]J. M. Kosterlitz, D. J. Thouless, and R. C. Jones, Phys. Rev. Lett. 36, 1217 (1976).
[13]A. J. Bray and M. A. Moore, J. Phys. C 14, 2629 (1981).
[14]We do not see the second peak in the $P(H)$ that J. R. L. deAlmeida and E. J. S. Lage [J. Phys. C 16, 939 (1983)] obtained for temperatures below but close to T_c. This is either due to the fact that the mean-field theory equations neglect the fluctuations or that $N \leq 400$ is still too small to observe this second peak.
[15]We define T_c as the lowest temperature at which (in an extrapolated thermodynamic limit) $Q = \sum_i m_i^2/N$ is nonzero. We find $T_c = 1.3$ for both the $S = 1$ XY and Heisenberg model.